

What is claimed is:

1. A computer-based method of generating a quantitative structure activity relationship comprising:
  - a) calculating a numerical representation of molecules consisting of  $n$  numbers per molecule; and,
  - b) estimating a probability distribution that a said molecules is active.
2. A method as recited in claim 1, wherein:
  - a) said estimating step is calculated with Bayes Theorem.
3. A method as recited in claim 1, wherein:
  - a) said probability distribution of said estimating step comprises  $n$  one-dimensional distributions.
4. A method as recited in claim 1, wherein:
  - a) said estimating step is performed by using a means to remove linear correlations between said  $n$  numbers per molecule.
5. A method as recited in claim 4, wherein:
  - a) said means to remove linear correlations between said  $n$  numbers per molecule is a principal components analysis.

6. A method as recited in claim 4, wherein:
- a) said means to remove linear correlations between said  $n$  numbers per molecule is a matrix diagonalization.
7. A method as recited in claim 1, wherein:
- 5 a) said estimating step is performed by using a means to remove dependencies between said  $n$  numbers per molecule.
8. A method as recited in claim 7, wherein:
- a) said means to remove dependencies between said  $n$  numbers per molecule is a principal components analysis.
- 10 9. A method as recited in claim 7, wherein:
- a) said means to remove dependencies between said  $n$  numbers per molecule is a matrix diagonalization.
10. A method as recited in claim 1, wherein:
- 15 a) said estimating step is performed by estimating a distribution over a single number.
11. A method as recited in claim 1, wherein:
- a) said estimating step is performed by replacing a single observation with a Gaussian distribution.